



U.S. Department of Energy

The Role of the Office of Science and AFCI

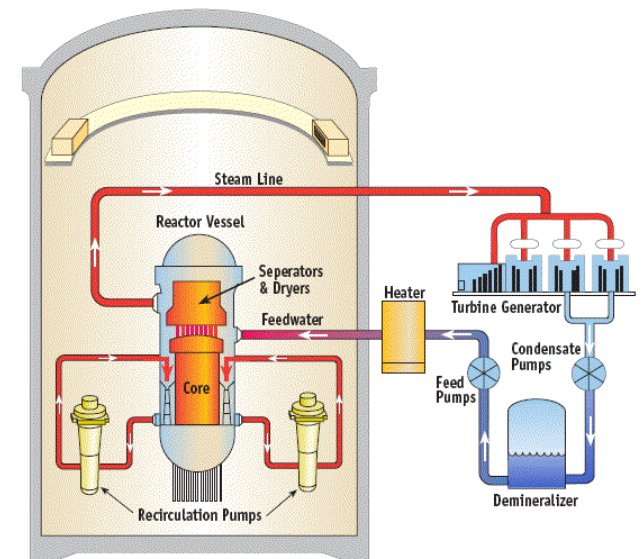
Global Nuclear Renaissance Summit

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Under Secretary for Science
U.S. Department of Energy
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www.science.doe.gov



Critical Role of Basic Science in AFCI and the Expansion of the U.S. Nuclear Energy Base

- What has changed in the last 30 years?
 - Science tools are improved – the computational facilities (massively parallel computers) and first principles science codes available today are a cornerstone of scientific discovery and industrial competitiveness
 - Continuing research under Advanced Fuel Cycle Initiative (AFCI) has led to an improved understanding of transuranic chemical separations – more economically viable
 - Transformational advances in materials science possible through improved analytical tools and research in nano-phase materials
- SC research critical to nuclear's long-term success
 - Pursue research now that will enable future growth and development
 - Engage next generation of scientists and engineers





Research Program Planning in Support of AFCI

3 Workshops Held in Summer of 2006

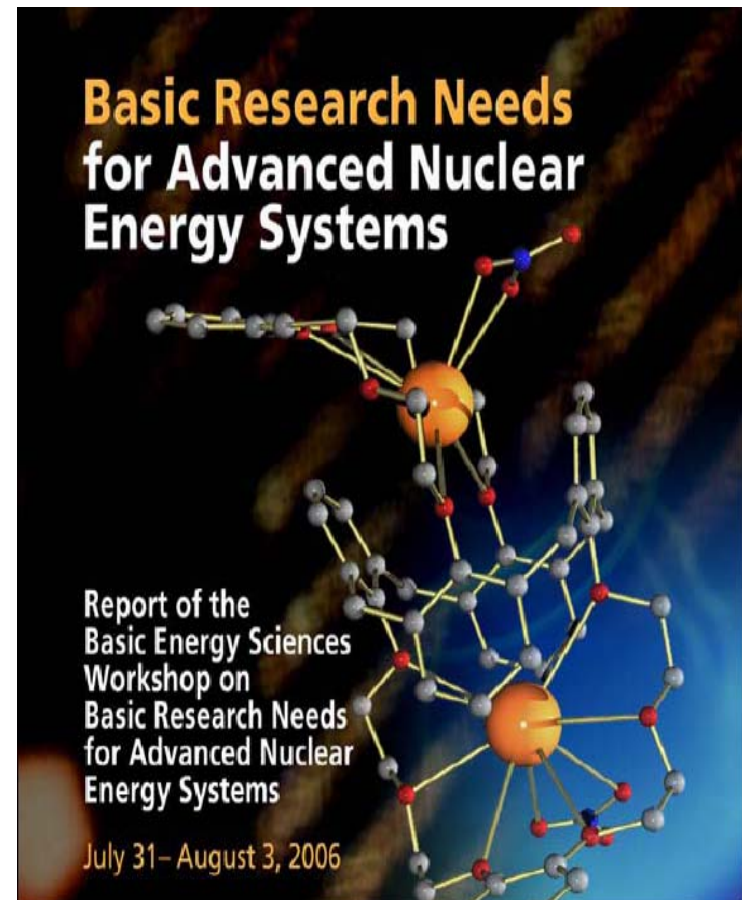
- Workshops
 - #1 - Basic Research Needs for Advanced Nuclear Energy Systems [Basic Energy Sciences (BES)]
 - #2 - Nuclear Physics and Related Computational Science R&D for Advanced Fuel Cycles [Nuclear Physics (NP) and Advanced Scientific Computing Research (ASCR)]
 - #3 - Simulation and Modeling for Advanced Nuclear Energy Systems [Nuclear Energy (NE) and Advanced Scientific Computing (ASCR)]
- Agenda
 - Industry (users), applied and basic research communities
 - Current state of the technology
 - Research opportunities
 - Reports available electronically (<http://www.science.doe.gov>)
- Attendance
 - Over 500 participants
 - Industry, universities, national laboratories, government agencies, and foreign collaborators
- Total of \$39.8M research funding available in FY '07



Workshop 1 (BES): Basic Research Needs for Advanced Nuclear Energy Systems (July 31 – August 3, 2006)

Fundamental challenge

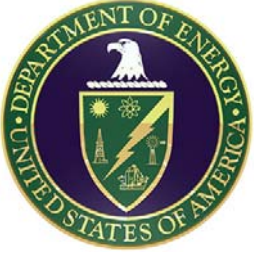
- Understand and control chemical and physical phenomena in multi-component systems from femto-seconds to millennia, at temperatures to 1000°C, and for radiation doses to hundreds of displacements per atom (dpa)
- www.sc.doe.gov/bes/reports/abstracts.html#ANES





Workshop 1 (BES): Key Issues

- Materials under extreme conditions over long exposure times
 - Advanced structural materials to withstand higher temperatures, higher radiation, and harsher chemicals
- Chemistry under extreme conditions over long exposure times
 - Chemistry in high-radiation environments, corrosive environments, at interfaces, and in complex solutions
- Separations science
 - f-electron interactions
 - Design molecules for separations
- Advanced actinide fuels
 - Development of actinide-containing fuels essential to closing nuclear fuel cycle
- Actinide containing waste forms
 - Challenge of dealing with new waste forms produced by actinide-containing fuels
- Dynamical measurements to understand fundamental physical and chemical phenomena
 - Improved methods for evaluation and use of nuclear data
- Predictive modeling and simulation
 - Multi-scale approaches for accurate models of relevant phenomena and complex systems across multiple length and time scales



Workshop 1 (BES): Status

- Solicitation for basic research proposals
 - understanding of nanoscale interactions under extreme conditions
 - mastering the behavior of actinides and of fission products
 - solution behavior under extreme conditions of radiation and temperature
 - interfacial behavior under extreme environmental conditions
- Pre-proposals are currently undergoing review.
- Encouragement for full proposal sent January 4, 2007
- Full proposals will be due March 14, 2007
- \$12.4 M to be awarded in FY '07



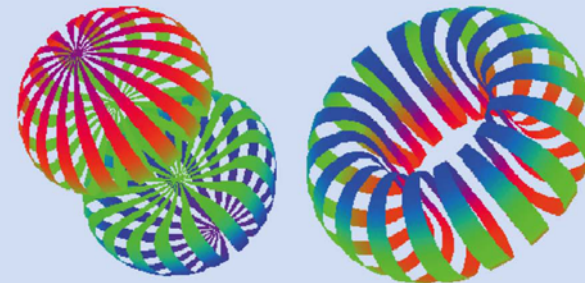
Workshop 2 [(NP) and (ASCR)]: Nuclear Physics and Related Computational Science R&D for Advanced Fuel Cycles (August 10-12, 2006)

Fundamental challenge

- Wall-to-wall simulation of the reactor core will require advanced nuclear theory calculations of relevant cross sections
- www.science.doe.gov/np/program/docs/AFC_Workshop_Report_FINAL.pdf

Report of the Nuclear Physics and Related Computational Science R&D for Advanced Fuel Cycles Workshop

Bethesda, Maryland



Co-sponsored by

Office of Nuclear Physics
Office of Advanced Scientific Computing Research
U.S. Department of Energy Office of Science

Co-chairs

Lee Schroeder
Ewing Lusk

August 10-12, 2006





Workshop 2 [(NP) and (ASCR)]: Key Issues

- Nuclear Measurements
 - High quality measurements, with both neutron and charged particle beams for a wide range of stable and radioactive nuclides)
 - Development and application of surrogate techniques to extract data where direct neutron measurement can not be applied
 - Strategic need for investment in facilities, experimental equipment and workforce
- Nuclear Data
 - Covariance data for evaluated nuclear data files
 - Further precision fast spectrum neutron cross-sections (fission, capture and scattering) for both major and minor actinides.
 - Inelastic cross sections for standard reactor structural materials
 - Consolidation of data for decay, delayed neutrons, fission yields and photon production
- Nuclear Theory and Computation
 - More fundamental and accurate description of nuclear reactions would help the NP, NE and science-based stockpile Stewardship programs
 - Advanced nuclear theory calculations of relevant cross sections where experimental evaluated data do not exist
 - Coordinated approach to integrate reaction-code components under one computational umbrella



Workshop 2 [(NP) and (ASCR)]: Status

- Solicitation for research proposals
 - help provide the nuclear data and knowledge
 - related theory efforts required for advanced nuclear fuel cycles
- www.science.doe.gov/grants/FAPN07-05.html
- Open until January 10, 2007
- \$2.4 M to be awarded in FY '07



Workshop 3 [(NE) and (ASCR)]: Simulation and Modeling for Advanced Nuclear Energy Systems (August 15-17, 2006)

Fundamental challenge

- Simulation of reactor systems to allow effective predictive tool for the complex properties of the fuels and materials over the operational lifetime
- www-fp.mcs.anl.gov/anes/





Workshop 3 [(NE) and (ASCR)]: Key Issues

- Users/community define accuracy and validation requirements
 - Advanced modeling and simulation can reduce development times of new fuel types and uncertainty in construction and development costs
 - Physics-based high-fidelity simulation codes can accelerate the licensing process, if regulatory process can allow simulation as a basis for risk analysis and design approvals
- Use DOE's large-scale facilities for proof-of-principle runs, development of new methods, and the production use of both existing and new tools Begin to develop next-generation simulation codes based on models closer to first principles aimed at deployment in the five to ten year time frame.
 - Current code base insufficiently predictive for long-term nuclear program goals but needed to address immediate design and planning needs
 - Open-source community codes
 - Build on experience and software from SciDAC (Scientific Discovery through Advanced Computing)
- Long-term research program aimed at advancing cross-cutting issues
 - Uncertainty quantification and error estimation
 - Multiscale and multiphysics codes scalable with fidelity for fundamental studies, design and engineering use
 - Engage university and laboratories to help train the next generation of computationally oriented nuclear engineers and scientists
- SC working with NE to incorporate the principles from the workshop into the applied R&D campaigns being planned by NE, and to ensure the platforms and cycle times are available
- \$25 M to be awarded in FY '07



Follow-On Workshops in Planning Stage:

Materials Under Extreme Conditions Workshop

Planned for June 10-14, 2007

- **Radiation Materials Science**
 - Development of radiation-tolerant materials
 - Application in fission, fusion, waste storage, high energy intensity processes, and defense applications over large dosage range, rate and duration
 - Understanding radiation damage mechanisms
- **Corrosion Science**
 - Effects of chemical and electrochemical environments on mass transport, chemistry and structural evolution
 - Application in nuclear energy, fossil fuel conversion plants, and industrial processes
 - Understanding mechanisms passive film breakdown, growth of localized corrosion sites, degradation in multiple exposure environments (e.g., combination of SCC and radiation)
- **Temperature Pressure and Strain Rates**
 - Effects of over wide range of temperatures and pressures, and strain rates from relatively static loadings in radioactive waste packages to very large in defense applications
 - Understanding the origins of strength and ductility, the degradation mechanisms as a function of the changing environment, and the behavior of novel materials such as molecular crystals, disordered systems, and nanoscale objects.
- **Magnetic and Electrical Fields**
 - Effects of changing fields on resistance, conductivity, ferroelectricity, and magnetoresistance properties
 - Understanding dielectric breakdown and similar phenomena in electrical conductors, resistors, and giant magnetoresistant materials.
- **Cross-cutting**
 - Opportunities that bridge experimental capabilities, theory, modeling and simulation capabilities



Summary

- Effective utilization of nuclear power will require continued improvements in nuclear technology
 - Basic research challenges represent some of the most demanding tests of our fundamental understanding of materials science and chemistry, our application of measurement techniques, and our ability to apply high end computational capabilities
 - Significant opportunities for advancing basic science with broad impacts for nuclear energy
- SC Research in Support of AFCI in FY '07
 - Basic Energy Sciences - \$12.4 million
 - Nuclear Physics - \$2.4 million
 - Advanced Scientific Computing Research - \$25 million

Additional Information

- www.science.doe.gov and look for the following Logo
- Links to SC Reports and other information

